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Stability and hyperfine structure of the four- and five-body muon-atomic clusters $a^+b^+\mu^-e^-$ and $a^+b^+\mu^-e^-e^-$.

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Abstract

Based on the results of accurate variational calculations we demonstrate stability of the five-body negatively charged ions $a^+b^+\mu^-e^-e^-$. Each of these five-body ions contains two electrons e^-, one negatively charged muon μ^- and two nuclei of the hydrogen isotopes $a, b = (p, d, t)$. The bound state properties of these five-body ions, including their hyperfine structure, are briefly discussed. We also investigate the hyperfine structure of the ground states of the four-body muonic quasi-atoms $a^+b^+\mu^-e^-$. In particular, we determine the hyperfine structure splittings for the ground state of the four-body muonic quasi-atoms: $p^+d^+\mu^-e^-$ and $p^+t^+\mu^-e^-$.

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I. INTRODUCTION

In our earlier work [1] we have discussed the four-body muonic quasi-atoms $a^+b^+\mu^-e^-$ and some of their properties. Here and everywhere below, the notations a and b stand for the nuclei of the hydrogen isoptopes (p designates protium, d is deuterium and t is tritium), μ^- (or μ) and e^- (or e) designate the negatively charged muon and electron, respectively. These muonic quasi-atoms are formed in liquid hydrogen/deuterium during muon-catalyzed fusion. It appears that the four-body muonic quasi-atoms, e.g, $p^+d^+\mu^-e^-, d^+d^+\mu^-e^-$, etc, have many extraordinary properties which follow from their two-shell cluster structure. In particular, each of these ions has a heavy central nucleus $ab\mu$ which is positively charged. Spatial radius of such a three-body nucleus is $R_\mu \approx \frac{a_0}{m_\mu}$. One electron moves around this heavy nucleus at disctances $R_e \approx a_0$, where a_0 is the Bohr radius. It is clear that $R_e \gg R_\mu$, since $\frac{m_\mu}{m_e} \approx 206.768$.

The two-shell cluster structure of these quasi-atoms allows one to predict a large number of their bound state properties without extensive numerical calculations. To check the overall accuracy of such predictions in [1] we have performed variational computations of the ground states in the six muonic atoms: $pp\mu e, pd\mu e, pt\mu e, dd\mu e, dt\mu e$ and $tt\mu e$. In such calculations we used the following particle masses $m_p = 1836.152701\ m_e$, $m_d = 3670.483014\ m_e$, $m_t = 5496.92158\ m_e$ and $m_\mu = 206.768262\ m_e$. These values of the particle masses are often used in recent computations of muonic molecular ions $ab\mu$ and other related systems. The same masses will be used in this study.

In this study we continue our analysis of the four-body quasi-atoms $a^+b^+\mu^-e^-$ and closely related five-body negatively charged ions $a^+b^+\mu^-e^-e^-$ (or $a^+b^+\mu^-e_2^-$). As follows from our preliminary evaluations (see below) the correspoding five-body negatively charged ions $a^+b^+\mu^-e^-e^-$ are stable and can be observed in actual experiments. These ions are of great interest for general theory of bound states in few-body systems with unit charges. In this study we want to investigate the stability of these five-body ions formed by the particles with unit charges. Another aim is to determine the hyperfine structure splitting of the ground states in the five-body $ab\mu e_2$ ions and four-body $ab\mu e$ hydrogen-like quasi-atoms. In particular, we discuss the hyperfine structure and determine the hyperfine structure splitting for the ground state of the $pd\mu e$ quasi-atom and predict the results of possible future experiements.

II. BOUND STATES IN THE FOUR-BODY MUONIC QUASI-ATOMS

In our variational calculations of the four-body quasi-atoms $a^+b^+\mu^-e^-$ in [1] we have applied the variational expansion written in the basis of the six-dimensional (or four-body) gaussoids of relative (or inter-particle) scalar coordinates r_{ij}. This variational expansion was originally proposed thirty years ago in [3] for accurate variational calculations of few-nucleon nuclei. For the bound $S(L=0)-$states the variational anzatz of six-dimensional (or four-body) gaussoids in relative coordinates is written in the form [3]

$$\Psi_{L=0} = \frac{1}{\sqrt{2}}(1+\delta_{ab}\epsilon_{ab}\mathcal{P}_{ab})\sum_{k=1}^{N} C_k \cdot exp(-\alpha_{12}^{(k)}r_{12}^2 - \alpha_{13}^{(k)}r_{13}^2 - \alpha_{23}^{(k)}r_{23}^2 - \alpha_{14}^{(k)}r_{14}^2 - \alpha_{24}^{(k)}r_{24}^2 - \alpha_{34}^{(k)}r_{34}^2) \quad (1)$$

where C_k are the linear coefficients (or linear variational parameters), while $\alpha_{ij}^{(k)}$ are the optimized non-linear parameters. The notation $\epsilon_{ab}\mathcal{P}_{ab}$ means the appropriate symmetrizer (or antisymmetrizer), i.e. a projection operator which produces the wave function with the correct permutation symmetry in those cases when $a=b$. This case is designated in Eq.(3) with the use of the delta-function. The operator $\mathcal{P}_{ab}$ is the pair-permutation operator for all coordinates, i.e. for the spatial, spin, iso-spin, etc, coordinates. In these calculations we have used two trial wave functions with $N=400$ and $N=600$ terms, respectively. All non-linear parameters $\alpha_{ij}^{(k)}$ in Eq.(3) have been varied carefully.

The results of new variational computations of the ground states in the six muonic quasi-atoms $pp\mu e, pd\mu e, pt\mu e, dd\mu e, dt\mu e$ and $tt\mu e$ can be found in Table I, where the total energies of these quasi-atoms are given in atomic units $\hbar=1, m_e=1, e=1$. These energies are slightly better than the analogous total energies obtained in [1]. In this study we need the improved total energies of the four-body muonic quasi-atoms $a^+b^+\mu^-e^-$ to show the stability of the corresponding five-body ions $a^+b^+\mu^-e^-e^-$ which contain two electrons (see below). Note also that there are twenty two bound states in the six three-body muonic molecular ions $pp\mu, pd\mu, pt\mu, dd\mu, dt\mu$ and $tt\mu$. Formally, each of these ions (in their ground and/or excited states) can bind an electron and form the four-body quasi-atom $ab\mu e$. In this study we restrict ourselves to the analysis of the six ground states only.

III. STABILITY OF THE FIVE-BODY MUONIC IONS

As follows from the general theory, the stability of the four-body quasi-atoms $a^+b^+\mu^-e^-$ means that the corresponding two-electron ions $a^+b^+\mu^-e^-e^-$ (or $a^+b^+\mu^-e_2^-$) are also stable. Each of these ions must have only one bound state which is, in fact, a weakly bound state, i.e. its binding energy is ≤ 1 % of its total energy. Here, the stability means the energy stability against the following two-particle dissociation into quasi-atom $ab\mu e$ and free electron

$$a^+b^+\mu^-e^-e^- = a^+b^+\mu^-e^- + e^- \tag{2}$$

Briefly, the word 'stability' means that the total energy of the five-body muonic ion $a^+b^+\mu^-e^-e^-$ is lower than the total energy of the four-body $a^+b^+\mu^-e^-$ quasi-atom in its ground state. Furthermore, the general theory of bound states in few-body systems predicts that the five-body $a^+b^+\mu^-e^-e^-$ ion has the only one bound $S(L=0)-$state and this state is a singlet electron state. Formally, such a state can be designated as the 1^1S_e-state, but in some cases this notation can lead to a confusion. In this Section we want to prove that the five-body negatively charged muonic ions $a^+b^+\mu^-e^-e^-$ are stable by performing accurate variational computations.

First, note that the bound (ground) state of the $a^+b^+\mu^-e^-e^-$ ion has the two-shell cluster structure. The internal three-body system, i.e. nucleus with electric charge +1, is formed by the three heavy particles a, b and μ. The spatial radius of such a 'quasi-nucleus' is $R_\mu \approx \frac{a_0}{m_\mu}$, where m_μ is the muon mass and a_0 is the Bohr radius. Everywhere below in this study we shall use only atomic units. In these units $\hbar = 1, e = 1$ and $m_e = 1$ and one finds $m_\mu = 206.768262$ and $a_0 = 1$. This means that $R_\mu \approx \frac{a_0}{206.768262} \ll a_0$. The two electrons are moving around the central, positively charged 'quasi-nucleus' at the distances $R_e \approx a_0 = 1$. In the zero-order approximation we can assume that $R_\mu = 0$ and $R_e = 1$. This leads us to the hydrogen-like quasi-atoms $ab\mu e$ and negatively charged ions $ab\mu ee$. However, even in this approximation we cannot ignore correlations between different particles, and first of all electron-muon correlations. In the next order approximation when $R_\mu > 0$ the situation becomes more complicated. This requires an additional flexibility of the variational anzatz which is used to construct trial wave functions. In all five-body calculations performed in this study we have used the variational anzatz which is written in the ten-dimensional

gaussoid functions (or five-body gaussoids) of the ten relative coordinates r_{ij} [3]

$$\Psi_{L=0} = (1 + \delta_{ab}\epsilon_{ab}\mathcal{P}_{ab})(1 + \mathcal{P}_{45}) \sum_{k=1}^{N} \sum_{(ij)=(12)}^{(45)} C_k \cdot exp(-\alpha_{ij}^{(k)} r_{ij}^2) \qquad (3)$$

where C_k are the linear coefficients (or linear variational parameters), while $\alpha_{ij}^{(k)} (= \alpha_{ji})$ are the optimized non-linear parameters. It is assumed in Eq.(3) that $i < j$. The notation $\mathcal{P}_{ab}$ means the permutation operator of the two particles a (particle 1) and b (particle 2). Additional phase $\delta_{ab}\epsilon_{ab} = \pm\delta_{ab}$, where δ_{km} is the Kronecker delta, is needed to provide the correct permutation symmetry in those systems where $a = b$. The analogous operator $\mathcal{P}_{45}$ is a pair permutation of the two identical electrons (particles 4 and 5) in the five-body $ab\mu ee$ ion. The overall electron symmetry of the trial wave function, Eq.(3), corresponds to the singlet electron state(s).

The results of numerical calculations of the ground state energies of the symmetric five-body ions $p^+p^+\mu^-e^-e^-, d^+d^+\mu^-e^-e^-$ and $t^+t^+\mu^-e^-e^-$ are shown in Table I. In these calculations we have used 400 basis functions in Eq.(3), i.e. $N = 400$. The same Table contains the total variational energies of the ground states of the symmetric four-body quasi-atoms: $p^+p^+\mu^-e^-, d^+d^+\mu^-e^-$ and $t^+t^+\mu^-e^-$ (see Section II). As follows from Table I the total energies of the five-body ions $p^+p^+\mu^-e^-e^-, d^+d^+\mu^-e^-e^-$ and $t^+t^+\mu^-e^-e^-$ are lower, i.e. they are more negative than the total energies of the corresponding four-body quasi-atoms $p^+p^+\mu^-e^-, d^+d^+\mu^-e^-$ and $t^+t^+\mu^-e^-$. Note again that in our four-body computations we have used the trial wave functions with $N = 400$ and 600 terms and all total energies of the five-body ions have been determined with the use of $N = 400$ basis functions, Eq.(3). This means the absolute stability of the five-body ions $a^+a^+\mu^-e^-e^-$ against dissociation as represented by Eq.(2). By performig analogous calculations for the corresponding five- and four-body non-symmetric ions $a^+b^+\mu^-e^-e^-$ and quasi-atoms $a^+b^+\mu^-e^-$ one finds that these ions are also stable.

Let us compare our results obtained for the five-body $a^+b^+\mu^-e^-e^-$ ions with the known total energies of the hydrogen atom H and hydrogen ion H^- with the infinitely heavy nucleus. Traditionally in atomic physics such systems are designated as the $^\infty$H atom and $^\infty H^-$ ion, respectively. The best-to-date variational energy obtained for the hydrogen $^\infty H^-$ ion [4] is -0.527 751 016 544 377 196 589 733 *a.u.*, where 21 - 22 decimal digits are stable. The total energy of the non-relativistic $^\infty$H atom is -0.5 *a.u.* (exactly). Therefore, the corresponding binding energy of the negatively charged hydrogen ion is $\approx$ -0.027751 *a.u.* Approximately

the same binding energy is obtained for each of the five-body ions $a^+a^+\mu^-e^-e^-$ considered here. In reality, one finds the two following differences between the hydrogen $^\infty H^-$ ion and five-body $a^+b^+\mu^-e^-e^-$ ion: (1) the mass of the central quasi-nucleus $a^+b^+\mu^-$ is always finite, and (2) there are correlations between electrons and heavy particles from the central quasi-nucleus. It is clear that the electron-muon correlations play the leading role here. In general, the contribution of such correlations slightly decreases the actual binding energy of the five-body $a^+b^+\mu^-e^-e^-$ ion.

IV. HYPERFINE STRUCTURE OF THE GROUND STATES OF THE FOUR-BODY QUASI-ATOMS

Now, consider the hyperfine structure splitting of the ground states in the four-body quasi-atoms $a^+b^+\mu^-e^-$ and five-body negatively charged ions $a^+b^+\mu^-e^-e^-$. Note, that the ground state of the five-body $a^+b^+\mu^-e^-e^-$ ion is the electron singlet state. The total electron spin of such a state equals zero exactly. Therefore, the electron spin does not contribute to the overall hyperfine structure. Briefly, we can say that the hyperfine structure of the five-body ion $a^+b^+\mu^-e^-e^-$ exactly coincides with the hyperfine structure of the three-body central 'quasi-nucleus' $a^+b^+\mu^-$. The hyperfine structures of the ground $S(L=0)-$states in six muonic molecular ions $a^+b^+\mu^-$ have been analyzed recently in [5].

In contrast with the five-body (two-electron) ions $a^+b^+\mu^-e^-e^-$, the corresponding four-body quasi-atoms have very interesting hyperfine structure. Below, in this study we restrict ourselves to the consideration of the $p^+d^+\mu^-e^-$ and $p^+t^+\mu^-e^-$ quasi-atoms. The proton, triton, muon and electron have spin equal $\frac{1}{2}$, while deuteron's spin equals 1. The dimension of the total spin-space for the $pd\mu e$ quasi-atom is $2\times 3\times 2\times 2=24$. The representation of the rotation group acting in this spin space is represented as the direct sum of the corresponding irreducible representations. The ranks of such irreducible representations essentially determine the hyperfine structure, while the differences between hyperfine energy levels can be obtained by solving the corresponding eigenvalue problem (all details can be found in [7]). The Hamiltonian $(\Delta H)_{h.s.}$ which represents the spin-spin interactions takes the following form (in atomic units) (see, e.g., [6])

$$(\Delta H)_{h.s.}=\frac{2\pi}{3}\alpha^2\frac{g_pg_d}{m_p^2}\langle\delta(\mathbf{r}_{pd})\rangle(\mathbf{s}_p\cdot\mathbf{s}_d)+\frac{2\pi}{3}\alpha^2\frac{g_pg_\mu}{m_pm_\mu}\langle\delta(\mathbf{r}_{p\mu})\rangle(\mathbf{s}_p\cdot\mathbf{s}_\mu)$$

$$+\frac{2\pi}{3}\alpha^2\frac{g_d g_\mu}{m_p m_\mu}\langle\delta(\mathbf{r}_{d\mu})\rangle(\mathbf{s}_d\cdot\mathbf{s}_\mu)+\frac{2\pi}{3}\alpha^2\frac{g_p g_e}{m_p}\langle\delta(\mathbf{r}_{pe})\rangle(\mathbf{s}_p\cdot\mathbf{s}_e)$$
$$+\frac{2\pi}{3}\alpha^2\frac{g_d g_e}{m_p}\langle\delta(\mathbf{r}_{de})\rangle(\mathbf{s}_d\cdot\mathbf{s}_e)+\frac{2\pi}{3}\alpha^2\frac{g_\mu g_e}{m_\mu}\langle\delta(\mathbf{r}_{\mu e})\rangle(\mathbf{s}_\mu\cdot\mathbf{s}_e) \quad (4)$$

where $\alpha=\frac{e^2}{\hbar c}$ is the fine structure constant, m_μ and m_p are the muon and proton masses, respectively. The factors g_μ, g_p, g_d and g_e are the corresponding $g-$factors. The expression for $(\Delta H)_{h.s.}$ is, in fact, an operator in the total spin space which has the dimension $(2s_p+1)(2s_d+1)(2s_\mu+1)(2s_e+1)=24$. In our calculations we have used the following numerical values for the constants and factors from Eq.(4): $\alpha=7.297352586\cdot10^{-3}, m_p=1836.152701m_e, m_\mu=206.768262m_e, g_e=$ -2.0023193043718 and $g_\mu=-2.0023218396$. The $g-$factors for the proton and deuteron are deteremined from the formulas: $g_p=\frac{\mathcal{M}_p}{I_p}$ and $g_d=\frac{\mathcal{M}_d}{I_d}$, where $\mathcal{M}_p=2.792847386$ and $\mathcal{M}_d=0.857438230$ are the magnetic moments (in nuclear magnetons) of the proton and deuteron, respectively. The spin of the proton and deuteron is designated in Eq.(4) as $I_p=\frac{1}{2}$ and $I_d=1$.

The energy levels of the hyperfine structure and the corresponding structure splittings (differences between energy levels) can be found in Table II. Note that these values are usually given in MHz, while the values of $(\Delta H)_{h.s.}$ which follow from Eqs.(4)) are expressed in atomic units. To re-calculate them from atomic units to MHz the conversion factor $6.57968392061\cdot10^9\ MHz/a.u.$ was used. The general hyperine structure of the ground state of the $pd\mu e$ quasi-atom follows from Table II. The total spin function has twenty four components. It can be represented as a direct sum of the following irreducible components (from the top to the bottom): (1) $J=\frac{3}{2}$ (four states), (2) $J=\frac{5}{2}$ (six states), (3) $J=\frac{1}{2}$ (two states), (4) $J=\frac{3}{2}$ (four states), (5) $J=\frac{1}{2}$ (two states), (6) $J=\frac{3}{2}$ (four states) and (7) $J=\frac{1}{2}$ (two states). The total final dimension of this direct sum is: $4+6+2+4+2+4+2=24$ as expected. The hyperfine structure splittings, i.e. the differences Δ, are shown in Table II. There are three large and three small Δ. In particular, the values of Δ_{12}, Δ_{34} and Δ_{67} are small. Very likely these differences are related with the protium-deuterium spin-spin interaction which is very small by its absolute value, since the expectation value of the proton-deuteron delta-function is very small [5]. On the other hand, the values of Δ_{23}, Δ_{45} and Δ_{56} are relativey large. They are related with the electron-nuclear, electron-muon and muon-nuclear spin-spin interactions. A slightly more contrast picture can be obtained for the ground states in other muonic quasi-atoms, e.g., $dt\mu e$ and $tt\mu e$. We have determined the hyperfine structures for the ground states in all six muonic quasi-atoms mentioned in

[1]. The hyperfine structure of the $pt\mu e$ quasi-atom can be found in Table III. In this case $g_t = \frac{\mathcal{M}_t}{I_t}$, where $\mathcal{M}_p = 2.792847386$ and $I_t = \frac{1}{2}$. The hyperfine structure of the $pd\mu e, pt\mu e$ and other similar quasi-atoms which contain Coulomb three-body quasi-nuclei $ab\mu$ must be confirmed in future experiments.

V. CONCLUSION

Thus, we have illustrated by numerical means the stability of the bound five-body ions $ab\mu ee$ in their ground states. Some of the properties of these five-body ions are also predicted. The hyperfine structure of these ions is identical to the hyperfine structure of the corresponing muonic molecular ions $ab\mu$. We also investigate the hyperfine structure of the four-body muonic quasi-atoms $ab\mu e$ which is substantially more complicated. To obtain this hyperfine structure splitting we have diagonalized the Hamiltonians of the spin-spin interactions which include six different terms and overall dimension up to 36 (for the $dd\mu e$ and $(dd\mu)^* e$ quasi-atoms). The hyperfine structure of the $pd\mu e$ and $pt\mu e$ quasi-atoms is investigated in details.

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[1] A.M. Frolov and D.M. Wardlaw, ArXiV: 1107.3768 [phys.,atom-ph.] (2011) (see also Phys. Rev. A **84**, 052507 (2011)).

[2] L.I. Men'shikov and L.N. Somov, Sov. Phys. Uspekhi **33**, 616 (1990).

[3] N.N. Kolesnikov and V.I. Tarasov, Yad. Fiz. **35**, 609 (1982), [Sov. J. Nucl. Phys. **35**, 354 (1982)] (see also the earlier references therein).

[4] A.M. Frolov, J. Phys. A: Math. Theor. **40**, 6175 (2007).

[5] A.M. Frolov, ArXiV: 1111.6351 [phys.,atom-ph.] (2011) and ArXiV: 1111.7056 [phys.,atom-ph.] (2011).

[6] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics: non-relativistic theory.*, (3rd. ed. Pergamon Press, New York (1976)), Chpt. XV.

[7] A.M. Frolov, Phys. Lett. A **357**, 334 (2006).

TABLE I: The total non-relativistic total energies E of the ground $S(L=0)-$states in the five-body ions $aa\mu ee$ and four-body quasi-atoms $aa\mu e$ (in atomic units).

	$pp\mu ee$	$dd\mu ee$	$tt\mu ee$
$E(N=400)$	-102.75052695	-110.34390610	-113.49923563
	$pp\mu e$	$dd\mu e$	$tt\mu e$
$E(N=400)$	-102.72331085	-110.31683802	-113.47266365
$E(N=600)$	-102.72332519	-110.31684129	-113.47266986
	$pd\mu e$	$pt\mu e$	$dt\mu e$
$E(N=400)$	-106.51226911	-107.99443693	-111.86419287
$E(N=600)$	-106.51233102	-107.99453043	-111.86421475

TABLE II: The hyperfine structure E_i and hyperfine structure splitting $\Delta_{i(i-1)}$ of the ground $S(L=0)-$state of the $pd\mu e$ quasi-atom (in MHz).

$E_i\ MHz$	$\Delta_{i(i-1)}\ MHz$
$\epsilon_{J=\frac{3}{2}}$ $1.2521503100\cdot10^7$	———-
$\epsilon_{J=\frac{5}{2}}$ $1.2517912194\cdot10^7$	$3.59090572\cdot10^3$
$\epsilon_{J=\frac{1}{2}}$ $9.3086776002\cdot10^6$	$3.209234594\cdot10^6$
$\epsilon_{J=\frac{3}{2}}$ $9.3043876675\cdot10^6$	$4.28993274\cdot10^3$
$\epsilon_{J=\frac{1}{2}}$ $-2.1222389818\cdot10^7$	$3.052677749\cdot10^7$
$\epsilon_{J=\frac{3}{2}}$ $-2.3095865825\cdot10^7$	$1.873476007\cdot10^6$
$\epsilon_{J=\frac{1}{2}}$ $-2.3100074249\cdot10^7$	$4.208423455\cdot10^3$

TABLE III: The hyperfine structure E_i and hyperfine structure splitting $\Delta_{i(i-1)}$ of the ground $S(L=0)-$state of the four-body $pt\mu e$ quasi-atom (in MHz).

	$E_i\ MHz$	$\Delta_{i(i-1)}\ MHz$
$\epsilon_{J=1}$	$1.5082272852\cdot10^7$	————
$\epsilon_{J=2}$	$1.5078349188\cdot10^7$	$3.9236642227\cdot10^3$
$\epsilon_{J=0}$	$1.6857006656\cdot10^6$	$1.3392648522\cdot10^7$
$\epsilon_{J=1}$	$1.6776620651\cdot10^6$	$8.0386005145\cdot10^3$
$\epsilon_{J=1}$	$-3.1838284105\cdot10^7$	$3.3515946170\cdot10^7$
$\epsilon_{J=0}$	$-3.1842399042\cdot10^7$	$4.1149362917\cdot10^3$